

# **Asian SEDPHAT Workshop: A workshop focused on ITC analysis**

Workshop at the Yokohama City University, Yokohama, September 13, 2012, co-organized by

## **The Japan Society for Calorimetry and Thermal analysis, BMIA Forum**

Organization committee: Susumu Uchiyama (Osaka University), Masayuki Oda (Kyoto Prefectural University), Fumio Arisaka (TIT)

- 9:30 – 10:00      **Registration**
- 10:00 – 10:10      **Welcome/Announcements**
- 10:10 - 11:30      **Mini-Symposium on ITC**
- Speakers: Shunichi Kidokoro (Nagaoka Tech. Univ.)**  
**Kohei Tsumoto (Tokyo Univ.)**  
**Chad Chad Brautigam (UT Southwestern, Dallas)**
- 11:30 - 12:00      **NITPIC: a New Integrator of Thermograms Produced by Isothermal Calorimetry**
- 12:00 - 13:00      **Lunch**

### **Data Analysis Workshop**

Lecturers: Chad Brautigam (UT Southwestern, Dallas), Rodolfo Ghirlando (NIH, Bethesda), Grzegorz Piszczek (NIH, Bethesda), Peter Schuck (NIH, Bethesda)

- 13:00 - 13:45      **Lecture: Basic introduction to SEDPHAT, NITPIC, GUSSI**
- SEDPHAT program structure
  - data files
  - fitting tools
  - concept of incompetent species and concentration errors
  - error bars in ITC isotherms
  - NITPIC vs ORIGIN: motivation and consequences
- 13:45 - 14:30      **Practical Exercise I**
- Integrate thermogram in NITPIC
  - loading single data set in SEDPHAT
  - setting data limits, removing bad data
  - fit single site mode
  - assessing success
  - saving results
  - plot results in GUSSI
- 14:30 - 15:00      **Lecture: Global modeling**
- Concept of global analysis
  - Global vs local parameters and incompetent fractions
  - Constraints

- Examples of multi-site models, competition models
- Linkage models (protonation, temperature, salt)
- Multi-method modeling

15:30 - 16:30

**Practical Exercise II**

- Mechanics of loading multiple data sets, setting constraints
- Example: two-site binding
- Example: competitive binding
- Example: three-component cooperative multi-site binding
- Example: protonation-linked binding
- Example: simple multi-method analysis

16:30 - 17:00

**Lecture: Statistics**

- Concept of error surface, methods of optimization
- Methods for confidence interval analysis
- Consequences of error bars of data points in ITC
- Simulation to predict significant experiments

17:00 - 17:30

**Practical Exercise III**

- Create error surface in 1d and 2d
- Confidence intervals by error surface projection
- Monte Carlo analysis